N-(4-Bromophenyl)urea 1967-25-5 | DTXSID30173337

Model Performance

Model	Data

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

Model Results

Predicted value: 1.98

Global applicability domain: Inside

Local applicability domain index: 5.90e-01

Confidence level: 7.27e-01

Nearest Neighbors from the Training Set

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3-Bromophenylurea Measured: 2.08 Predicted: 1.98

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N-(4-Bromophenyl)urea Measured: 1.98 Predicted: 1.98

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(3-Methyl-4-bromophenyl)urea

Measured: 2.49 **Predicted:** 2.03

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3-Chlorophenylurea Measured: 1.82 Predicted: 1.93

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(2-Chlorophenyl)urea Measured: 1.27 Predicted: 1.76